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NEWS	8	FEB	16	INSPEC Adding Its Own IPC codes and Author's E-mail Addresses
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NEWS	10	APR	02	PATDPAFULL: Application and priority number formats enhanced
NEWS	11	APR	02	
NEWS			02	
NEWS	13	APR	02	
NEWS	14	APR	07	
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NEWS	16	APR	07	
NEWS	17	JUN	16	WPI First View (File WPIFV) will no longer be available after July 30, 2010
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NEWS	19	JUN	18	CAS and FIZ Karlsruhe announce plans for a new STN platform
NEWS	20	JUN	18	IPC codes have been added to the INSPEC backfile (1969-2009)
NEWS	21	JUN	21	Removal of Pre-IPC 8 data fields streamline displays in CA/Caplus, CASREACT, and MARPAT
NEWS	22	JUN	21	Access an additional 1.8 million records exclusively enhanced with 1.9 million CAS Registry Numbers
NEWS	23	JUN	28	EMBASE Classic on STN Introducing "CAS Chemistry Research Report": 40 Years of Biofuel Research Reveal China Now Atop U.S. in

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NEWS 24 JUN 29 Enhanced Batch Search Options in DGENE, USGENE,
and PCTGEN

NEWS EXPRESS FEBRUARY 15 10 CURRENT WINDOWS VERSION IS V8.4.2, AND CURRENT DISCOVER FILE IS DATED 15 JANUARY 2010.

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 TOTAL

 ENTRY
 SESSION

 FULL ESTIMATED COST
 0.22
 0.22

FOLL ESTIMATED COST U.2

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STRUCTURE FILE UPDATES: 15 JUL 2010 HIGHEST RN 1232397-02-2 DICTIONARY FILE UPDATES: 15 JUL 2010 HIGHEST RN 1232397-02-2

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http://www.cas.org/support/stngen/stndoc/properties.html

-

Uploading C:\Program Files\Stnexp\Queries\10574995\Struc 1.str

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chain nodes: 12 \quad 3 \quad 4 \quad 5 \quad 6 \quad 7 \quad 8 \quad 14 \quad 15 \quad 16 \quad 22 ring nodes: 10 \quad 11 \quad 12 \quad 13 \quad 17 \quad 18 \quad 19 \quad 20 \quad 21 chain bonds: 1-2 \quad 1-3 \quad 1-4 \quad 1-5 \quad 4-6 \quad 6-7 \quad 7-8 \quad 8-9 \quad 8-14 \quad 11-15 \quad 15-16 \quad 16-17 \quad 16-22 ring bonds: 9-10 \quad 9-13 \quad 10-11 \quad 11-12 \quad 12-13 \quad 17-18 \quad 17-21 \quad 18-19 \quad 19-20 \quad 20-21 exact/norm bonds: 1-2 \quad 1-3 \quad 1-4 \quad 1-5 \quad 4-6 \quad 6-7 \quad 7-8 \quad 8-9 \quad 8-14 \quad 9-10 \quad 9-13 \quad 10-11 \quad 11-12 \quad 11-15 \quad 17-12 \quad 18-19 \quad 19-20 \quad 20-21
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### G1:C, N

Match level:
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:Atom
10:Atom 11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom
19:Atom 20:Atom 21:Atom 22:CLASS

#### STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1

G1 C, N

Structure attributes must be viewed using STN Express query preparation.

=> 11

SAMPLE SEARCH INITIATED 12:53:01 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -2 TO ITERATE

100.0% PROCESSED

2 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01 FULL FILE PROJECTIONS:

ONLINE \*\*COMPLETE\*\* BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: PROJECTED ANSWERS:

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0 SEA SSS SAM L1

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100.0% PROCESSED 36 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 191.54 191.76

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FILE COVERS 1907 - 16 Jul 2010 VOL 153 ISS 4
FILE LAST UPDATED: 15 Jul 2010 (20100715/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2010
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CAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2010.

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http://www.cas.org/legal/infopolicv.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER:
                        2005:324136 CAPLUS
DOCUMENT NUMBER:
                          142:402927
TITLE:
                         Sequence selective pyrrole and imidazole polyamide
                          metal complexes for targeting therapeutic or
                         diagnostic groups to polynucleotides
INVENTOR(S):
                         Jaramillo, David; Brodie, Craig; Howard, Warren;
                          Taleb, Robin; Aldrich-Wright, Janice
PATENT ASSIGNEE(S):
                         University of Western Sydney, Australia
SOURCE:
                         PCT Int. Appl., 97 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:
                         Patent
LANGUAGE:
                         English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
     PATENT NO.
                 KIND DATE APPLICATION NO. DATE
     WO 2005033077
                      A1 20050414 WO 2004-AU1368 20041007
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             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
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PRIORITY APPLN. INFO.:
                                           AU 2003-905512
                                                               A 20031007
                                                               W 20041007
                                           WO 2004-AU1368
                        CASREACT 142:402927; MARPAT 142:402927
OTHER SOURCE(S):
    The present invention relates to the preparation of platinum-group metal
     complexes with sequence selective pyrrole and imidazole polyamide compds.
     for targeting therapeutic or diagnostic groups to polynucleotides. More
     particularly, the present invention relates to sequence selective
     targeting of metal complexes, such as metallodrugs and metallodiagnostics,
     to polynucleotides. For example, N-[5-[5-(2-aminoethylcarbamoy1)-2-methyl-
     1H-pyrryl-3-ylcarbamoyl]-1-methyl-2H-pyrrol-3-yl]-1-methyl-1H-imidazole-2-
     carboxamide (L) was prepared in a multistep process and reacted with
     trans-Pt(NH3)2Cl2 to give trans-PtL(NH3)2Cl. The affinity consts. of
     trans-PtL(NH3)2C1 with duplex DNA were determined A pharmaceutical composition
     containing a complex such as trans-PtL(NH3)2Cl can be used to treat cancer,
     HIV and hepatitis C or as a diagnostic.
                              THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
OS.CITING REF COUNT:
                        1
                               (1 CITINGS)
REFERENCE COUNT:
                         14
                              THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
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COST IN U.S. DOLLARS
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CA SUBSCRIBER PRICE
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http://www.cas.org/support/stngen/stndoc/properties.html

=> d scan

- L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- IN 1H-Pyrrole-2-carboxylic acid, 1-methyl-4-[[(1-methyl-4-nitro-1H-pyrrol-2-y1)carbonyl]amino]-, methyl ester
- MF C13 H14 N4 O5

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT \*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- IN 1H-Imidazole-2-carboxamide, N-[5-[[[5-[[(2-aminoethyl)amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-1-methyl-
- MF C19 H24 N8 O3

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):54

- L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- IN Ruthenium, (2,2'-bipyridine-kN1,kN1')dicarbonyldichloro-
- MF C12 H8 C12 N2 O2 Ru
- CI CCS

- \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*
- L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- yı)carbonyıjamınoj-iH-imidazole-z-carboxamidejjtetraamminedichiorod.
  (9CI)
- MF C54 H77 C12 N27 O11 Pt2
- CI CC:

PAGE 1-A

$$\begin{array}{c} \text{NH}_3 \\ \\ \text{Pt} \\ \hline \\ \text{C1}^- \end{array}$$

PAGE 1-B

Me----

PAGE 1-C

PAGE 2-C

L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN Ethanone, 2,2,2-trichloro-1-(1-methyl-1H-imidazol-2-yl)-MF C6 H5 C13 N2 O

Page 12

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- IN Ruthenium(2+), (5-chloro-1,10-phenanthroline-N1,N10)bis(1,10-
- phenanthroline-N1,N10)-, (OC-6-33)-, bis[hexafluorophosphate(1-)] (9CI) MF C36 H23 Cl N6 Ru . 2 F6 P

CM 1

CM 2

- L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- IN 1H-Pyrrole-2-carbonyl chloride, 1-methyl-4-nitro-

Page 13

MF C6 H5 C1 N2 O3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN http://dimethylethoxylocarboxylicacid, 4-[[[4-[[4-[[4-[[4-[[4-[4]]]amino]-1-methyl-1H-imidazol-2-y1]carbonyl]amino]-1-methyl-1H-imidazol-2-y1]carbonyl]amino]-1-methyl-1H25 N9 06

C20 H25 N9 06

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN 1H-Imidazole-2-carboxylic acid, 1-methyl-MF C5 H6 N2 O2

CI COM

56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

Platinum(1+),  $[N-[5-[[[6-(amino-\kappa N)hexyl]amino]carbonyl]-1-methyl-1H-$ IN pyrrol-3-yl]-1-methyl-4-[[(1-methyl-1H-pyrrol-2-yl)carbonyl]amino]-1Hpyrrole-2-carboxamide]diamminechloro-, chloride, (SP-4-2)- (9CI)

C24 H39 C1 N9 O3 Pt . C1 MF

CI CCS

● c1-

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN L7 Platinum, diamminedichloro-, (SP-4-2)-ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT MF C12 H6 N2 Pt

CCS, COM

- \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*
- L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- IN 1H-Imidazole-2-carboxylic acid, 4-[[(1,1-dimethylethoxy)carbonyl]amino]-1methyl-, methyl ester C11 H17 N3 O4

ME

## Page 15

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN IN 1H-Pyrrole-2-carboxylic acid, 1-methyl-4-nitro-

C6 H6 N2 O4 MF

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 1-methyl-4-[[[1-methyl-4-[[(1-methyl-1H-

pyrrol-2-yl)carbonyl]amino]-1H-pyrrol-2-yl]carbonyl]amino]-, methyl ester C19 H21 N5 O4

MF

L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 4-nitro-, methyl ester

MF C6 H6 N2 O4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN lH-Imidazole-2-carboxylic acid, 4-[[[4-[[(1,1-dimethylethoxy)carbonyl]amino]-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1, ethyl ester

MF C22 H29 N9 O6

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Ruthenium

MF Ru

CI COM

Ru

#### Page 17

L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN 1H-Pyrrole-2-carboxylic acid, 1-methyl-4-[[(1-methyl-1H-pyrrol-2-yl)carbonyl]amino]-

MF C12 H13 N3 O3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Platinum

MF Pt

CI COM

Рt

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- IN Carbamic acid, [2-[[[1-methyl-4-[[(1-methyl-4-nitro-1H-pyrrol-2-yl)carbonyl]amino]-1H-pyrrol-2-yl]carbonyl]amino]ethyl]-,

1,1-dimethylethyl ester (9CI)

MF C19 H26 N6 O6

- L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- IN 1H-Pyrrole-2-carboxylic acid, 1-methyl-

```
Page 18
```

- 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- IN Platinum(1+), diamminechloro[1,1-dimethylethyl [6-(amino-kN)hexyl]carbamate]-, (SP-4-2)- (9CI)
- MF C11 H30 C1 N4 O2 Pt
- CI CCS, COM

$$\begin{array}{c|c} & \text{NH3} & \text{O} \\ & 2+ \\ -\text{C1-Pt} & \text{NH2-(CH2)6-NH-C-OBu-t} \\ & \text{NH3} \end{array}$$

- 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN L7
- IN Methanesulfonic acid, 1,1,1-trifluoro-
- C H F3 O3 S MF
- CI COM

- L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- IN 1H-Imidazole-2-carboxylic acid, 4-[[(1,1-dimethylethoxy)carbonyl]amino]-1methyl-
- C10 H15 N3 O4 MF

- L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- 2,2'-Bipyridine IN C10 H8 N2
- MF
- CI COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- IN 1H-Imidazole-2-carboxylic acid, 1-methyl-4-nitro-, ethyl ester
- MF C7 H9 N3 O4

- 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN L7
- Ethane, 1,1',1''-[methylidynetris(oxy)]tris-C7 H16 O3 IN
- MF
- CI COM

OEt

EtO-CH-OEt

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- IN Ruthenium, dichlorobis(1,10-phenanthroline-κN1,κN10)-
- MF C24 H16 C12 N4 Ru
- CI CCS, COM

- L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- IN Platinum(1+), [N-[5-[[[2-(amino-KN)ethyl]amino]carbonyl]-1-methyl-1Hpyrrol-3-yl)-1-methyl-4-[([1-methyl-1H-imidazol-2-yl)carbonyl]amino]-1Hpyrrole-2-carboxamide]diamminechloro-, chloride, (SP-4-2) (9CI)
- MF C19 H30 C1 N10 O3 Pt . C1
- CI CCS

c1-

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- IN Carbamic acid, N-(2-aminoethyl)-, 1,1-dimethylethyl ester
- MF C7 H16 N2 O2
- CI COM

- 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- TN κN) ethyl amino | carbonyl | ethyl | amino | carbonyl | -1-methyl -1H-pyrrol -3yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1Hpyrrol-2-yl]amino]carbonyl]-1-methyl-1H-imidazol-4-yl]amino]-4oxobutyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-4-hydroxy-1-methyl-1H-pyrrol-3-yl]-1-methyl-4-[[(1-methyl-1H-imidazol-2vl)carbonyl]amino]-1H-imidazole-2-carboxamide]diamminechloro- (9CI)
- C54 H70 C1 N24 O11 Pt MF
- ccs

PAGE 1-A

$$\begin{array}{c} \text{NH}_3 \\ \text{-C1-Pt} & \text{NH}_2-\text{CH}_2-\text{CH}_2-\text{NH}-\text{C}-\text{CH}_2-\text{CH}_2-\text{NH}-\text{C} \\ \text{NH}_3 & \text{O} \end{array}$$

PAGE 1-B

PAGE 2-B

L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Carbamic acid, N-(6-aminohexy1)-, 1,1-dimethylethyl ester MF C11 H24 N2 O2

MF C11 H24 N2 CI COM

O || t-BuO-C-NH-(CH2)6-NH2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 56 ANSMERS REGISTRY COPYRIGHT 2010 ACS on STN

Ruthenium(2+), [2-[(1,10-phenanthrolin-5-y1-kN1,kN10) oxy]ethanamine]bis(1,10-phenanthroline-kN1,kN10)-, (CC-6-33)-, bis[hexafluorophosphate(1-)] (9CI)

MF C38 H29 N7 O R u. 2 F6 P

CM 1

CM 2

#### Page 24

56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN 1H-Imidazole-2-carboxylic acid, 1-methyl-, ethyl ester

MF C7 H10 N2 O2

CI COM

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN L7

DO ANSWERS REGISTAL OPERIOR 2010 ACS ON SIN Ruthenium (2+), (2,2'-bipyridine-kN1, kN1')dicarbonyl (10,11,12,13-tetrahydrodipyrido[3,2-a:2',3'-c]phenazine-kN4, kN5)-, bis[hexafluorophosphate(1-)] (9CI) C30 H22 N6 O2 Ru. 2 F6 P IN

CM 1

CM 2 Page 25

L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Dicarbonic acid, C,C'-bis(1,1-dimethylethyl) ester

MF C10 H18 O5

CI COM

t-BuO-C-O-C-OBu-t

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN 1H-Imidazole-2-carboxylic acid, 1-methyl-4-[[(1-methyl-1H-imidazol-2-

yl)carbonyl]amino]-, methyl ester

MF C11 H13 N5 O3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Ruthenium, dicarbonyldichloro-

MF C2 C12 O2 Ru

CI CCS, COM

- L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
  IN 1H-Imidazole-2-carboxylic acid, 4-[[[4-[[(1,1dimethylethoxy)carbonyl]amino]-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1methyl-
- MF C15 H20 N6 O5

- L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- IN Platinum, diamminedichloro-, (SP-4-1)-
- MF C12 H6 N2 Pt
- CI CCS, COM

- \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*
- L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- pyrrol-2-yl)carbonyl]amino]-1H-pyrrol-2-yl]carbonyl]amino]-
- MF C18 H19 N5 O4

- L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- 1H-Pyrrole-2-carboxylic acid, 1-methyl-4-nitro-, methyl ester IN C7 H8 N2 O4

- L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- 1H-Pyrrole-2-carboxylic acid, 1-methyl-4-[[(1-methyl-1H-pyrrol-2-IN yl)carbonyl]amino]-, methyl ester
- MF C13 H15 N3 O3

L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Nitric acid

MF H N O3

CI COM

о— и— он

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN 1H-Imidazole-2-carboxylic acid, 4-[[[4-[[(1,1-dimethylethoxy)carbonyl]amino]-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-, ethyl ester

MF C17 H24 N6 O5

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Rhodium

MF Rh

CT COM

Rh

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Dipyrido[3,2-a:2',3'-c]phenazine, 10,11,12,13-tetrahydro-

MF C18 H14 N4

Page 29

CI COM

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- IN Palladium
- MF Pd
- CI COM

Pd

- L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- IN Carbamic acid, [2-[[[1-methyl-4-[[1-methyl-4-[[(1-methyl-1H-imidazol-2-yl)carbonyl]amino]-1H-pyrrol-2-yl]carbonyl]amino]-1H-pyrrol-2-
- yl]carbonyl]amino]ethyl]-, 1,1-dimethylethyl ester (9Cl) MF C24 H32 N8 O5

- \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*
- L7 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

#### Page 30

IN 1,10-Phenanthroline, 4-chloro-ME C12 H7 C1 N2

CI COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN Ruthenium, (2,2'-bipyridine-  $\kappa N1,\kappa N1')$  dicarbonylbis(trifluoromethanesulfonato- $\kappa O)$ -IN (9CI)
- C14 H8 F6 N2 O8 Ru S2 MF
- CCS

- 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- IN 1H-Imidazole, 1-methyl-
- MF C4 H6 N2
- CI COM



- 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN L7
- IN 1H-Imidazole-2-carboxylic acid, 4-amino-1-methyl-, ethyl ester
- MF C7 H11 N3 O2
  - COM

H<sub>2</sub>N

- \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*
- 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- IN 1,6-Hexanediamine
- MF C6 H16 N2
- COM

H2N- (CH2)6-NH2

- \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*
- 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN L7
- 1H-Pyrrole-2-carboxylic acid, 1-methyl-4-[[(1-methyl-4-nitro-1H-pyrrol-2vl)carbonvl]amino]-
- MF C12 H12 N4 O5

- \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*
- 56 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN L7
- TN 1,2-Ethanediamine
- MF C2 H8 N2
- COM

 ${\rm H_2N-CH_2-CH_2-NH_2}$ 

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

#### ALL ANSWERS HAVE BEEN SCANNED

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COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.49	220.27
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chain nodes: 12 \quad 3 \quad 4 \quad 5 \quad 6 \quad 7 \quad 8 \quad 14 \quad 15 \quad 16 \quad 22 ring nodes: 10 \quad 11 \quad 12 \quad 13 \quad 17 \quad 18 \quad 19 \quad 20 \quad 21 chain bonds: 1-2 \quad 1-3 \quad 1-4 \quad 1-5 \quad 4-6 \quad 6-7 \quad 7-8 \quad 8-9 \quad 8-14 \quad 11-15 \quad 15-16 \quad 16-17 \quad 16-22 ring bonds: 9-10 \quad 9-13 \quad 10-11 \quad 11-12 \quad 12-13 \quad 17-18 \quad 17-21 \quad 18-19 \quad 19-20 \quad 20-21 exact/norm bonds: 1-2 \quad 1-3 \quad 1-4 \quad 1-5 \quad 4-6 \quad 6-7 \quad 7-8 \quad 8-9 \quad 8-14 \quad 9-10 \quad 9-13 \quad 10-11 \quad 11-12 \quad 11-15 \quad 17-12 \quad 18-19 \quad 19-20 \quad 20-21
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### G1:C, N

Match level:
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:Atom
10:Atom 11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom
19:Atom 20:Atom 21:Atom 22:CLASS

#### L8 STRUCTURE UPLOADED

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G1 C, N

Structure attributes must be viewed using STN Express query preparation.

=> 18

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100.0% PROCESSED 2 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01 FULL FILE PROJECTIONS:

ONLINE \*\*COMPLETE\*\* BATCH \*\*COMPLETE\*\* 2 TO 124

PROJECTED ITERATIONS: PROJECTED ANSWERS:

0 TO

0 SEA SSS SAM L8

=> 18 full

FULL SEARCH INITIATED 12:58:54 FILE 'REGISTRY' 36 TO ITERATE FULL SCREEN SEARCH COMPLETED -

100.0% PROCESSED 36 ITERATIONS 9 ANSWERS

SEARCH TIME: 00.00.01

L10 9 SEA SSS FUL L8

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE

TOTAL.

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FILE LAST UPDATED: 15 Jul 2010 (20100715/50)
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CAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2010.

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=> 110 L11 3 L10

=> d ibib abs hitstr 1-3

L11 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2007:460473 CAPLUS

DOCUMENT NUMBER: 147:66212

TITLE: Synthesis of DNA-sequence-selective hairpin polyamide

platinum complexes

AUTHOR(S): Taleb, Robin I.; Jaramillo, David; Wheate, Nial J.;

Aldrich-Wright, Janice R.

CORPORATE SOURCE: School of Biomedical and Health Sciences, University

of Western Sydney, Penrith Sout DC, NSW, Australia SOURCE: Chemistry-A European Journal (2007), 13(11),

3177-3186

CODEN: CEUJED: ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Two DNA-sequence-selective hairpin polyamide platinum(II) complexes, containing pyrrole and imidazole heterocyclic rings, have been synthesized by

different methods. A six-ring complex, selective for (A/T)GGG-(A/T) DNA

CN

sequences, was made by using solid-phase synthesis, while an eight-ring complex, selective for (A/T)CCTG(A/TP) DNA sequences, was made by utilizing standard wet chemical Solid-phase synthesis resulted in a significantly higher yield, required less purification and is more efficient than the wet synthesis; as such, it is the preferred method for further work. The metal complexes were characterized by IH and 195Pt NMR spectroscopy and ESI mass spectrometry. The two compds. provide a foundation for the synthesis of more complex mols. containing multiple hairpins and/or platinum groups.

IT 940956-91-2P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(synthesis of DNA-sequence-selective hairpin polyamide platinum complexes)

RN 940956-91-2 CAPLUS

940936-91-2 CAPUS
Platinum(1+), [N-[5-[[5-[[4-[[2-[[5-[[5-[[5-[[5-[[3-[[3-(amino-kN)propyl]amino]-3-exepropyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pirnol-3-yl]amino]carbonyl]-1-methyl-1H-pirnol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-1-methyl-pyrrol-3-yl]-1-methyl-1H-pyrrol-3-yl]-1-methyl-1H-pyrrol-3-yl]-1-methyl-1H-pyrrol-3-yl]-1-methyl-1H-pyrrol-3-yl]-1-methyl-1H-pyrrol-3-yl]-1-methyl-1H-pyrrol-3-yl]-1-methyl-1H-pyrrol-3-yl]-1-methyl-1H-pyrrol-3-yl]-1-methyl-1H-pyrrol-3-yl]-1-methyl-1H-pyrrol-3-yl]-1-m

PAGE 1-A

PAGE 1-B

PAGE 2-A

OS.CITING REF COUNT:

THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2006:619875 CAPLUS

DOCUMENT NUMBER: 145:264972

TITLE: Polyamide Platinum Anticancer Complexes Designed to Target Specific DNA Sequences

AUTHOR(S): Jaramillo, David; Wheate, Nial J.; Ralph, Stephen F.;

Howard, Warren A.; Tor, Yitzhak; Aldrich-Wright,

Janice R.

CORPORATE SOURCE: School of Biomedical and Health Sciences, University of Western Sydney, Campbelltown, 2560, Australia

SOURCE: Inorganic Chemistry (2006), 45(15), 6004-6013

CODEN: INOCAJ; ISSN: 0020-1669 PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:264972 AB

Two new platinum complexes, trans-chlorodiammine[N-(2-aminoethyl)-4-[4-(Nmethylimidazole-2-carboxamido)-N-methylpyrrole-2-carboxamido]-Nmethylpyrrole-2-carboxamidelplatinum(II) chloride (DJ1953-2) and trans-chlorodiammine[N-(6-aminohexyl)-4-[4-(N-methylimidazole-2carboxamido)-N-methylpyrrole-2-carboxamido]-N-methylpyrrole-2carboxamide]platinum(II) chloride (DJ1953-6) have been synthesized as proof-of-concept mols. in the design of agents that can specifically target genes in DNA. Coordinate covalent binding to DNA was demonstrated with electrospray ionization mass spectrometry. Using CD, these complexes were found to show greater DNA binding affinity to the target sequence: d(CATTGTCAGAC)2, than toward either d(GTCTGTCAATG)2, which contains different flanking sequences, or d(CATTGAGAGAC)2, which contains a double base pair mismatch sequence. DJ1953-2 unwinds the DNA helix by around 13°, but neither metal complex significantly affects the DNA melting temperature Unlike simple DNA minor groove binders, DJ1953-2 is able

inhibit, in vitro, RNA synthesis. The cytotoxicity of both metal complexes in the L1210 murine leukemia cell line was also determined, with D1953-6 (34 µM) more active than D31953-2 (>50 µM). These results demonstrate the potential of polyamide platinum complexes and provide the structural basis for designer agents that are able to recognize biol. relevant sequences and prevent DNA transcription and replication.

IT 906675-13-6P, DJ 1953-2

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (USes) (preparation of DJ1953-2)

RN 906675-13-6 CAPLUS

CN Platinum(1+), [N-[5-[[[2-(amino-KN)ethyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-1-methyl-4-[[(1-methyl-1H-imidazol-2-yl)carbonyl]amino]-1H-pyrrole-2-carboxamide]diamminechloro-, chloride, (SP-4-2)- (9CI) (CA INDEX NAME)

● C1-

IT 906675-14-7P, DJ 1953-6 RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of DJ1953-6)

RN 906675-14-7 CAPLUS

CN Platinum(1+), [N-[5-[[[6-(amino-κN)hexyl]amino]carbonyl]-1-methyl-1Hpyrrol-3-yl]-1-methyl-4-[[(1-methyl-1H-imidazol-2-yl)carbonyl]amino]-1Hpyrrole-2-carboxamide]diamminechloro-, chloride, (SP-4-2)- (9CI) (CA INDEX NAME)

● C1-

OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD (8 CITINGS)

REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD, ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2005:324136 CAPLUS

DOCUMENT NUMBER: 142:402927

TITLE: Sequence selective pyrrole and imidazole polyamide

metal complexes for targeting therapeutic or

diagnostic groups to polynucleotides

INVENTOR(S): Jaramillo, David; Brodie, Craig; Howard, Warren;

Taleb, Robin; Aldrich-Wright, Janice
PATENT ASSIGNEE(S): University of Western Sydney, Australia

SOURCE: PCT Int. Appl., 97 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA7	ENT :	NO.			KIN	D	DATE		- 2	APPL	ICAT:	ION I	NO.		D	ATE	
WO	0 2005033077			A1		2005	20050414		WO 2004-AU1368					20041007			
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KΕ,	KG,	KP,	KR,	ΚZ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
		ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
		AZ,	BY,	KG,	ΚZ,	MD,	RU,	ΤJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
		EE,	ES,	FΙ,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,
		SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,
		SN,	TD,	TG													
AU	AU 2004278050			A1	1 20050414				AU 2004-278050				20041007				
EP	EP 1678133				A1	A1 20060712			1	EP 2004-761403				20041007			

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR CN 1863771 Α 20061115 CN 2004-80029402 20041007 ZA 2006003288 Α 20070926 ZA 2006-3288 20041007 NZ 546896 NZ 2004-546896 Α 20041007 US 20070265240 A1 20071115 US 2007-574995 20070306 PRIORITY APPLN. INFO .: AU 2003-905512 20031007 20041007

WO 2004-AU1368
OTHER SOURCE(S): CASREACT 142:402927; MARPAT 142:402927

The Present invention relates to the preparation of platinum-group metal complexes with sequence selective pyrrole and imidazole polyamide compds. for targeting therapeutic or diagnostic groups to polynucleotides. More particularly, the present invention relates to sequence selective targeting of metal complexes, such as metallodrugs and metallodiagnostics, to polynucleotides. For example, N-[5-[5-(2-aminoethylcarbamoyl)-2-methyl-1H-pyrryl-3-ylcarbamoyl]-1-methyl-2H-pyrrol-3-yl]-1-methyl-1H-inidazole-2-carboxemide (L) was prepared in a multistep process and reacted with trans-Ptt(NH3)2Cl2 to give trans-Ptt(NH3)2Cl2. The affinity consts. of trans-Ptt(NH3)2Cl2 with duplex DNA were determined A pharmaceutical composition containing a complex such as trans-Ptt(NH3)2Cl can be used to treat cancer, HIV and hepatitis C or as a diagnostic.

IT 849665-10-7P 906675-13-6P RL: CPS (Chemical process), DSN (Diagnostic use); PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); BTOL (Biological study); PREP

(Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP
(Preparation); PROC (Process); USES (Uses)
 (preparation and binding consts. with DNA as anti-AIDS/antiviral/antitumor

agents/diagnostic agents) RN 849665-10-7 CAPLUS

Note 19905 10 CAL Model
Platinum(1+), [N-[5-[[[6-(amino-kN)hexyl]amino]carbonyl]-1-methyl-1Hpyrrol-3-yl]-1-methyl-4-[[(1-methyl-1H-pyrrol-2-yl)carbonyl]amino]-1Hpyrrol-2-carboxamide]diamminechloro-, chloride, (SP-4-2)- (9CI) (CA
INDEX NAME)

€ c1 =

RN 906675-13-6 CAPLUS

Platinum(1+),  $[N-[5-[[[2-(amino-\kappa N)]ethy1]amino]carbony1]-1-methy1-1H-$ 

pyrrol-3-y1]-1-methy1-4-[[(1-methy1-1H-imidazol-2-y1)carbony1]amino]-1Hpyrrole-2-carboxamide]diamminechloro-, chloride, (SP-4-2)- (9CI) (CA INDEX NAME)

● c1=

IT 849665-18-5P 849665-19-6P
RL: DGN (Diagnostic use); PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of platinum-group metal complexes with sequence selective pyrrole/imidazole polyamides as anti-AIDS/antiviral/antitumor agents/diagnostic agents)

RN 849665-18-5 CAPLUS

CN

PAGE 1-A

$$\begin{array}{c} \text{NH}_3 \\ \\ \text{Pt} \\ \hline \\ \text{C1}^- \end{array}$$

PAGE 1-B

Me----

PAGE 1-C

PAGE 2-C

RN 849665-19-6 CAPLUS

Platinum(1+), [N-[5-[[[5-[[[4-[[2-[[[5-[[[5-[[[5-[[[2-[[12-(mino-kN)ethyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-2-yl]amino[carbonyl]-1-methyl-1H-pyrrol-2-yl]amino[carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-4-hydroxy-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-4-hydroxy-1-methyl-1H-pyrrol-3-yl]-1-methyl-4-[[(1-methyl-1H-imidazol-2-yl)carbonyl]amino]-1H-imidazol-2-yl)carbonyl]amino]-1H-imidazol-2-carboxamide]diamminechloro- (9CI) (CA INDEX NAME)

CN

PAGE 1-A

$$\begin{array}{c} & & & & & \\ & & & & \\ NH_3 & & & & \\ -C1-Pt & & NH_2-CH_2-CH_2-NH-C-CH_2-CH_2-NH-C \\ & & & NH_3 & & & \\ NH_3 & & & & & \\ \end{array}$$

PAGE 1-B

PAGE 2-B

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